

# Calculated NMR Parameters (Chemical Shifts and Coupling Constants) of Cyclic $C_4H_2$ and $C_4H_4$ Molecules Containing Carbene Centers, and of Some of their Boron Analoga, Using Density Functional Theory (DFT)

Bernd Wrackmeyer

Anorganische Chemie II, Universität Bayreuth, D-95440 Bayreuth, Germany

Reprint requests to Prof. Dr. B. Wrackmeyer. E-mail: b.wrack@uni-bayreuth.de

Z. Naturforsch. **59b**, 37–43 (2004); received October 24, 2003

Singlet state structures of small, cyclic hydrocarbons which can result from the addition of molecular dicarbon ( $C_2$ ) to ethyne ( $HC\equiv CH$ ) or ethene ( $H_2C=CH_2$ ) have been calculated (B3LYP/6-311+G(d,p) level of theory), and were found to contain carbene centres. Some structures of analogous boranes (replacement of the carbene centers by BH fragments) were also calculated. The computation of NMR parameters such as chemical shifts  $\delta^{13}C$  and  $\delta^{11}B$ , and coupling constants  $^1J(^{13}C, ^1H)$ ,  $^1J(^{11}B, ^1H)$ ,  $J(^{13}C, ^{13}C)$  and  $J(^{13}C, ^{11}B)$  shows that these data can be used for the discussion of the bonding situation. The presence of inverted carbene centers is clearly indicated by the increased  $^{13}C$  nuclear magnetic shielding. Scalar  $^{13}C$ - $^{13}C$  spin-spin coupling involving carbene centers are frequently dominated by spin-dipole and spin-orbital interactions.

*Key words:* Carbenes, Cyclic Hydrocarbons, Boranes, MO Calculations, NMR Parameters